Applicant: Steven D. Lacy et al.

Serial No.: 09/420,334 Filed: October 18, 1999

Page: 2

76. The computer program product of claim 26, wherein:

each of the sources has a associated set of source properties describing the source; and the instructions operable to cause a programmable processor to define the sources include instructions operable to cause a programmable processor to receive for each of the sources a set of values for one or more of the source properties associated with the source.

77. The computer program product of claim 54, wherein:

at least one of the source properties is selected from the group consisting of molecular weight, equivalents, density and concentration.

78. The computer program product of claim 54, wherein:

at least one of the course properties is a type describing a class of chemicals to be used in generating the library design.

79. A computer-implemented method for generating a library design for a combinatorial library of materials, a combinatorial library being a collection of two or more members that contain some variance in chemical composition, chemical amount, reaction conditions, and/or processing conditions, a member being a single position in a library, the library design being electronic data representing one or more components distributed across a conceptual arrangement of cells representing a combinatorial library, the cells corresponding to members of the combinatorial library and/or locations on a physical substrate, the method comprising:

defining a set of one or more parameters to be used in preparing the combinatorial library, each parameter being electronic data being electronic data corresponding to a process condition to be applied to one or more cells of the arrangement representing the combinatorial library;

defining one or more parameter values for each of the set of parameters, the parameter values representing an amount of the corresponding process condition to be applied to one or more of the cells of the arrangement, such that the parameter values for at least one of the set of parameters vary between a minimum amount and a maximum amount; and

R

BE

Applicant: Steven D. Lacy et al.

Serial No.: 09/420,334 Filed

: October 18, 1999

Page 3

generating a data file defining the library design, the data file comprising electronic data representing the one or more components distributed across the conceptual arrangement of cells representing the combinatorial library, the parameters and the parameter values.

- 80. The method of claim 79, wherein the parameter values for at least one of the parameters are defined to vary over time and or across two or more cells in the arrangement.
- 81. The method of claim 79, wherein the parameter values for at least one of the parameters vary according to a gradient selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.
- 82. The method claim 7\(\mathfrak{f}\), wherein the parameter values for at least one of the parameters correspond to amounts of a process condition selected from the group consisting of temperature, pressure, time, flow rate and stirring speed.
- 83. The method claim 79, further comprising: generating a graphical representation of the library design, the graphical representation describing parameter values assigned to one or more of the cells in the arrangement for one or more of the parameters.
- 84. The method claim 79, further comprising: using the data file to cause an automated apparatus to prepare the combinatorial library according to the library design.
- 85. A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, a combinatorial library being a collection of two or more members that contain some variance in chemical composition, chemical amount, reaction conditions, and/or processing conditions, a member being a single position in a library, the library design being electronic data representing one or more components distributed across a conceptual arrangement of cells representing a combinatorial library, the cells corresponding to members of the combinatorial library and/or locations on a physical substrate, the product



Applicant: Steven D. Lacy et al.

Serial No.: 09/420,334 Filed

: October 18, 1999

Page

comprising instructions operable to cause a programmable processor to:

define a set of one or more parameters to be used in preparing the combinatorial library. each parameter being electronic data being electronic data corresponding to a process condition to be applied to one or more cells of the arrangement representing the combinatorial library;

define one or more parameter values for each of the set of parameters, the parameter values representing an amount of the corresponding process condition to be applied to one or more of the cells of the arrangement, such that the parameter values for at least one of the set of parameters vary between a minimum amount and a maximum amount; and

generate a data file defining the library design, the data file comprising electronic data representing the one or more components distributed across the conceptual arrangement of cells representing the combinatofial library, the parameters and the parameter values.

- The computer program product of claim 85, wherein the parameter values for at least one 86. of the parameters are defined to vary over time and/or across two or more cells in the arrangement.
- 87. The computer program product claim 85, wherein the parameter values for at least one of the parameters vary according to a gradient selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.
- 88. The computer program product of claim 85, wherein the parameter values for at least one of the parameters correspond to amounts of a process condition selected from the group consisting of temperature, pressure, time, flow rate and stirring speed.
- 89. The computer program product of claim 85, further comprising instructions operable to cause a programmable processor to:

generate a graphical representation of the library design, the graphical representation describing parameter values assigned to one or more of the cells in the arrangement for one or more of the parameters.

90. The computer program product of claim 85, further comprising instructions operable to

